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Stereo sensitivity of exchange interactions in Ni^{II} and Cu^{II} heterospin complexes with 5-formylpyrrolyl-substituted nitroxides

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Abstract

© 2016, Springer Science+Business Media New York.5-Formylpyrrolyl-substituted nitronyl and imino nitroxide radicals HL1 and HL2 were synthesized. Their solid phases are formed by packing pairs of the molecules. In the {HL1..HL1} pairs, the dominant interaction is the ferromagnetic exchange with J/kB = 8.8 K (Hamiltonian H= 2 J(s1→ · s2→)). The ferromagnetic exchange occurs also in the heterospin molecules [Ni(L1)2], [Cu(L1)2], and [Ni(L2)2(MeOH)2]. In the complexes [Ni(L1)2] and [Cu(L1)2], a small change in the mutual orientation of the coordinated ligands has a considerable effect on the value and the sign of the energy of exchange interactions between the unpaired electrons of the metal ion and paramagnetic ligands.

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Keywords

copper(II) complexes, nickel(II) complexes, nitroxide radicals, pyrrole, quantum chemical calculations, X-ray diffraction